PhD grant ANR COSMOS

New approaches based on ion mobility coupled to mass spectrometry for the analysis of supramolecular polymers

Keywords: Mass spectrometry, Ion mobility, Supramolecular polymers, Isomers, Sequencing.

Laboratory: Laboratoire Analyse et Modélisation pour la Biologie et l'Environnement (LAMBE),
CNRS UMR 8587. Université d'Evry-Paris Saclay
Building Maupertuis, 1er étage, Bd François Mitterrand 91025 EVRY CEDEX
http://www.lambe.univ-evry.fr
X: @LAMBE_UMR8587

Scientific context and objectives

This doctoral project is within the framework of the ANR project COSMOS. This project aims to develop innovative analytical methods based on the ion mobility-mass spectrometry coupling (IM-MS) to characterize supramolecular polymers. These assemblies can, for example, regulate numerous functions in life processes, or also to serve as sensors or catalysts. In this context, the polymer chemistry team (ECP) at IPCM, partner of this project, developed supramolecular helical assemblies composed of 1,3,5-benzene tricarboxamide (BTA) monomers as a scaffold for cooperative catalysis. Nevertheless, such edifices of more and less large sizes, and involving, by definition, non-covalent interactions are particularly delicate to analyze with common analytical techniques (FT-IR, UV, CD, SAXS and SANS). Moreover, to date, no state-of-the-art technique has been introduced to precisely characterize the local structure e.g. the sequence of each monomer and the relative orientation of the distinct peripheral side chains.

Proposed approach and available resources

The development of innovative methodologies based on IM-MS coupling making it possible to probe and discriminate various BTA based supramolecular architectures is the core of this project. Firstly, conditions for preparation/analysis of BTA homo-assemblies will be screened and optimised. The homo-assemblies will be more finely characterized by studying influence of grafting of different functional groups, to obtain a distribution of conformational isomers according to their shape and size. Finally, approach will be extended to hetero-assemblies with variable length and composition. The final objectives of this project are both to develop a precise and robust sequencing method, but also to establish a cartographic database allowing to highlight both sequential and/or conformational isomers. The gained fingerprints, can be used to correlate sample preparation (structure/composition of BTA) with catalysis results. This project will be carried out in close collaboration with the two other partners involved into the project: Drs Matthieu Raynal/Laurent Bouteiller (Institut Parisien De Chimie Moléculaire (IPCM; UMR 8232 CNRS CNRS/Sorbonne Université, Paris) and Drs Roberto Lazzaroni/Patrick Brocorens (Université de Mons), for the synthesis/characterisation of these assemblies in solution and for molecular modelling, respectively.
The host laboratory (LAMBE, Université d'Evry Paris-Saclay, Evry-Courcouronnes) has seven mass spectrometers on site, among them one of which will be particularly used for the project: a SELECT SERIES Cyclic IMS ion mobility instrument with different ionisation sources.
The main activity of the project will take place within LAMBE (Evry), but occasional stays within IPCM (Paris) are expected to carry out the synthesis of some functionalized BTA monomers and solution characterization of the resulting supramolecular assemblies (FTIR, CD, SAXS et SANS).

Applicant profile

The applicant should have a background in chemistry, ideally in analytical chemistry. Prior experience in mass spectrometry and skills in one of the following areas: analytical chemistry, and/or polymer chemistry would be highly appreciated. The candidate should have a 5-year degree (Master 2 or engineering school) and evidences of scientific English skills (writing and oral communication). The candidate is expected to have good writing and communication skills and an ability to work in a multidisciplinary team. Thoroughness, curiosity and autonomy are essential for this project.

Full description of the project can be accessed on adum.fr.

Description of funding: The PhD grant is supported by the ANR COSMOS.
Duration of funding: 36 months.
Application deadline: 30/09/2024.
Expected starting date: 01/10/2024.
PhD supervisor: Cédric Przybylski (cedric.przybylski@univ-evry.fr).
PhD Co-supervisor: William Buchmann (william.buchmann@univ-evry.fr).
Application process: Applications must be deposited on ADUM: https://adum.fr/candidature/
They must include a detailed CV, Master's grades (M1 and M2), one or two recommendation letters from direct supervisors (M1 and M2 internships) and a cover letter describing your motivations for the project.